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=> d que l22
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                LEWIS ACID"+PFT/CT
L6         5455 SEA FILE=HCAPLUS ABB=ON  PLU=ON  LEWIS ACIDS+NT/CT
L14             STR
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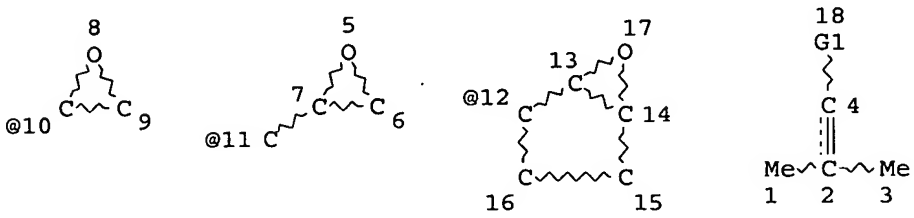


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VAR G1=11/10/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE
L16         965 SEA FILE=REGISTRY SSS FUL L14
L17         107 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16(L)(RACT OR RGT OR RCT)/RL

L18           3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND (L5 OR L6 OR LEWIS)
L21           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND ?LUMIN?
L22           4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 OR L21


=> d l22 ibib abs hitind hitstr 1-4

L22  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2004:751588  HCAPLUS
DOCUMENT NUMBER:          141:379730
TITLE:                    Towards a total synthesis of quinocarcin:
                          Diastereoselective synthesis of functionalized
                          azepino[1,2-b]isoquinolines
AUTHOR(S):                Koepler, Oliver; Laschat, Sabine; Baro, Angelika;
                          Fischer, Peter; Miehlich, Burkhard; Hotfilder, Marc;
                          le Viseur, Christoph
CORPORATE SOURCE:         Institut fuer Organische Chemie der Technischen
                          Universitaet Braunschweig, Braunschweig, 38106,
                          Germany
SOURCE:                   European Journal of Organic Chemistry (2004), (17),
                          3611-3622
                          CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER:                Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
GI
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,3-Disubstituted tetrahydro-oxazolo-isoquinolinones I (R = α-CO2Et or β-CO2Et) were obtained from phenylalanine in seven steps and 42% overall yield by Katritzky's benzotriazole method. The tricyclic oxazolidinone I (R = α-CO2Et) was further converted into amino alc. II (R = α-CH2OMe) by employing a chemoselective reduction of the ester group with LiBH4/MeOH. Compound II (R = α-CH2OMe) and the corresponding 1-unsubstituted tetrahydroisoquinoline alc. II (R = H) were converted into aldehydes III and IV, which cyclized in the presence of different **Lewis** acids to give the substituted azepino[1,2-b]isoquinolines V and VI, resp., which are key structural features of the alkaloid quinocarcin (VII). The stereoselectivities of the **Lewis**-acid-catalyzed heteroene reaction are highly dependent on the substitution pattern and the type of **Lewis** acid.

CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 27

ST asym synthesis azepinoisoquinoline **Lewis** acid catalyzed heteroene cyclization quinocarcin; antitumor agent human Ewing's sarcoma azepinoisoquinoline quinocarcin

IT Cyclization catalysts
(**Lewis** acid-catalyzed hetero-ene cyclization catalysts; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

IT Addition reaction catalysts
(ene, **Lewis** acid-catalyzed hetero-ene cyclization catalysts; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

IT Addition reaction
(ene, stereoselective, **Lewis** acid-catalyzed hetero-ene cyclization; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

IT Cyclization
(stereoselective, **Lewis** acid-catalyzed hetero-ene cyclization; diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

IT 2510-33-0P 215928-81-7P 219640-74-1P 223460-44-4P 782500-81-6P
782500-84-9P 782500-85-0P 782500-86-1P 782500-87-2P
782500-89-4P 782500-90-7P 782500-91-8P 782500-92-9P
782500-93-0P 782500-95-2P 782500-96-3P 782500-97-4P 782501-01-3P
782501-02-4P 782501-04-6P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

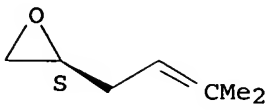
IT 109-63-7 563-43-9, **Ethylaluminum** dichloride, reactions
7550-45-0, Titanium tetrachloride, reactions 7646-78-8, Tin tetrachloride, reactions 7646-85-7, Zinc (II) chloride, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

IT **782500-89-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(diastereoselective synthesis of functionalized azepino[1,2-b]isoquinolines)

RN 782500-89-4 HCAPLUS

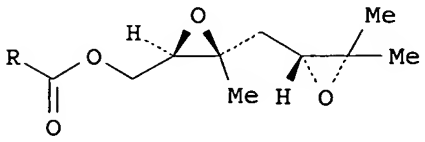
CN Oxirane, (3-methyl-2-butenyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

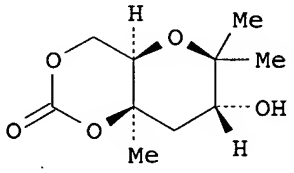


REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

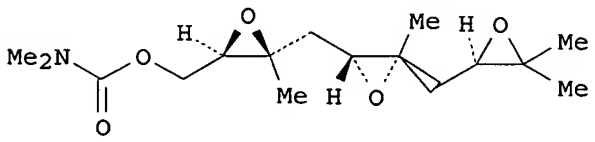
L22 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:385564 HCAPLUS
DOCUMENT NUMBER: 139:117351
TITLE: Biomimetic Synthesis of Fused Polypyrans: Oxacyclization Stereo- and Regioselectivity Is a Function of the Nucleophile
AUTHOR(S): Bravo, Fernando; McDonald, Frank E.; Neiwert, Wade A.; Do, Bao; Hardcastle, Kenneth I.
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (2003), 5(12), 2123-2126
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:117351
GI



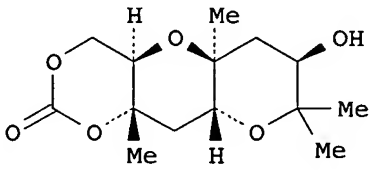
I



II



III



IV

AB The stereoselectivity of **Lewis** acid-induced endo-regioselective oxacyclizations of 1,4-diepoxides is dependent upon the nature of the terminating nucleophile. For instance, ring-opening/recyclization of the carbonate-substituted diepoxide I (R = Me3CO) provides a cis-fused bicyclic product II, whereas carbamate-derived I (R = Me2N) affords the

trans-fused diastereomer of II. Stereospecific and regioselective conversion of the tertiary carbamate-terminated 1,4,7-triepoxide III to tricyclic all-trans-fused polypyran IV is also demonstrated.

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **565183-88-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(allylic oxidation; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

IT 565183-76-8P 565183-77-9P 565183-78-0P 565183-80-4P 565183-82-6P 565183-84-8P 565183-90-6P 565183-91-7P **565183-92-8P** **565183-93-9P** **565183-94-0P** 565183-95-1P 565183-96-2P 565183-98-4P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

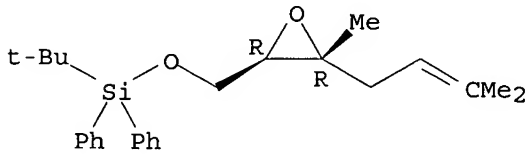
IT 43161-23-5P **565183-74-6P** **565183-79-1P** **565183-81-5P** **565183-83-7P** 565183-89-3P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(epoxidn.; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

IT **565183-88-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(allylic oxidation; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

RN 565183-88-2 HCAPLUS

CN Silane, (1,1-dimethylethyl)[[(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methoxy]diphenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

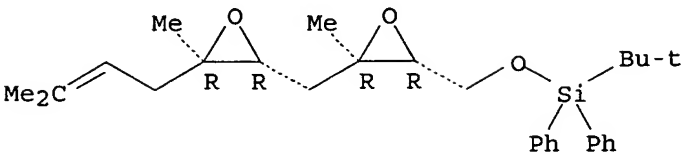


IT **565183-92-8P** **565183-93-9P** **565183-94-0P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)

RN 565183-92-8 HCAPLUS

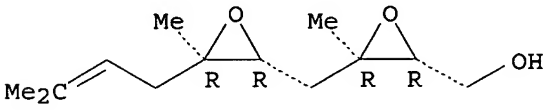
CN L-gluco-Heptitol, 2,3:5,6-dianhydro-4,7-dideoxy-1-O-[(1,1-dimethylethyl)diphenylsilyl]-3-C-methyl-6-C-(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



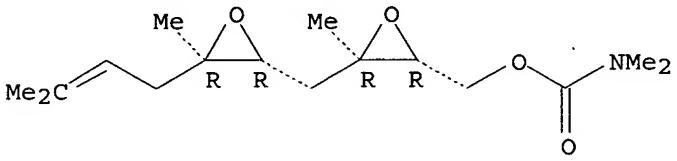
RN 565183-93-9 HCAPLUS
CN L-gluco-Heptitol, 2,3:5,6-dianhydro-4,7-dideoxy-3-C-methyl-6-C-(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



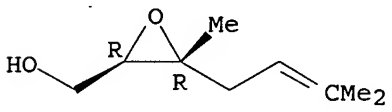
RN 565183-94-0 HCAPLUS
CN L-gluco-Heptitol, 2,3:5,6-dianhydro-4,7-dideoxy-3-C-methyl-6-C-(3-methyl-2-butenyl)-, dimethylcarbamate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



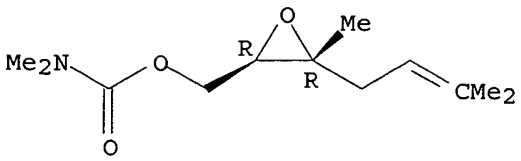
IT **565183-74-6P 565183-79-1P 565183-81-5P**
565183-83-7P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(epoxidn.; biomimetic synthesis of pyranodioxanes, furanopyrans and pyranopyrans via regio- and stereoselective ring opening/oxacyclization of carbonate- and carbamate-derivatized diepoxides and triepoxides)
RN 565183-74-6 HCAPLUS
CN Oxiranemethanol, 3-methyl-3-(3-methyl-2-butenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



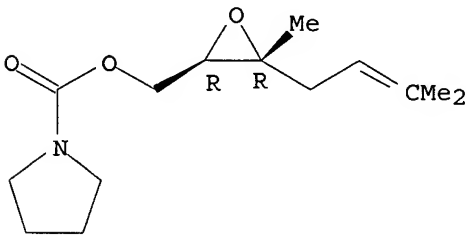
RN 565183-79-1 HCAPLUS
CN Carbamic acid, dimethyl-, [(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



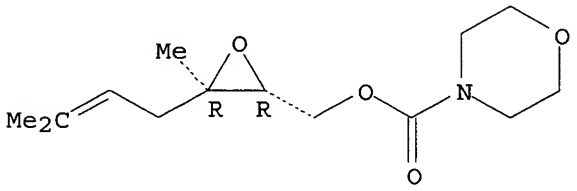
RN 565183-81-5 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, [(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 565183-83-7 HCAPLUS
CN 4-Morpholinecarboxylic acid, [(2R,3R)-3-methyl-3-(3-methyl-2-butenyl)oxiranyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

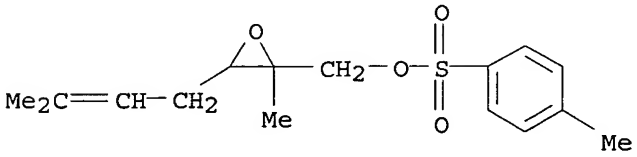


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

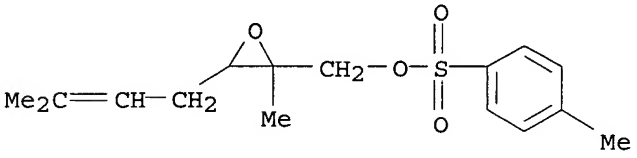
L22 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:538472 HCAPLUS
DOCUMENT NUMBER: 119:138472
TITLE: A tellurium transposition route to allylic alcohols: overcoming some limitations of the Sharpless-Katsuki asymmetric epoxidation
AUTHOR(S): Dittmer, Donald C.; Discordia, Robert P.; Zhang, Yanzhi; Murphy, Christopher K.; Kumar, Archana; Pepito, Aurora S.; Wang, Yuesheng
CORPORATE SOURCE: Cent. Sci. Technol., Syracuse Univ., Syracuse, NY, 13244, USA
SOURCE: Journal of Organic Chemistry (1993), 58(3), 718-31
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:138472
AB Good yields of enantiomeric allylic alcs. can be obtained in high enantiomeric excess (ee) by combining the Sharpless-Katsuki asym. epoxidn. process (SAE) with tellurium chemical The advantages of the tellurium process are as follows: (1) the 50% yield limitation on the allylic alc. in the Sharpless kinetic resolution (SKR) can be overcome; (2) allylic tertiary alcs. which are unsatisfactory substrates in the SKR can be obtained in high optical purity; (3) optically active secondary allylic alcs. with tertiary alkyl substituents (e.g. tert-butyl) at C-1 can be obtained in high ee; (4) optically active sterically congested cis secondary alcs. can be obtained in high ee; and (5) the nuisance of the slow SAE of some vinyl carbinols can be avoided. The key step in the reaction sequence is either a stereospecific 1,3-transposition of double bond and alc. functionalities or an inversion of the alc. configuration with concomitant deoxygenation of the epoxide function in epoxy alcs. Trans secondary allylic alcs. can be converted to cis secondary allylic alcs. by way of erythro epoxy alcs. (glycidols); threo glycidyl derivs. are converted to trans secondary allylic alcs. These transformations are accomplished by the action of telluride ion, generated in situ from the element, on a glycidyl sulfonate ester. Reduction of elemental Te is conveniently done with rongalite (HOCH2SO2Na) in an aqueous medium. This method is satisfactory when Te2- is required to attack a primary carbon site of a glycidyl sulfonate. In cases where Te2- is required to attack a secondary carbon site, reduction of the tellurium must be done with NaBH4 or LiEt3BH. Elemental tellurium is precipitated during the course of the reactions
and can be recovered and reused.
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 26
IT **80232-50-4P 80287-12-3P** 111321-48-3P 121401-06-7P
121468-44-8P 121958-41-6P 131750-35-1P 131750-36-2P 131750-37-3P
131750-38-4P 131831-36-2P 131831-37-3P 131831-38-4P 131831-39-5P
147048-00-8P 147048-01-9P 147048-07-5P 147048-10-0P 147048-16-6P
147127-69-3P 147127-70-6P 147127-73-9P 147127-79-5P 147127-80-8P
147493-35-4P 200205-69-2P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction of, with telluride ion)
IT 147048-17-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of, with lithium **aluminum** hydride)
IT 62777-71-3P, (2R,3R)-2,3-Epoxygeraniol 78513-12-9P **80232-49-1P**
80299-55-4P 82188-73-6P 84039-81-6P 89194-12-7P
97589-09-8P 107033-45-4P 107796-93-0P 114180-68-6P 114180-70-0P
147047-99-2P 147048-15-5P 147048-20-2P 147127-72-8P 147127-74-0P
147127-77-3P 147127-81-9P 147129-38-2P 147600-50-8P 161511-98-4P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and tosylation of)
IT 18448-47-0, Methyl 1-cyclohexene-1-carboxylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, with lithium **aluminum** hydride)
IT **80232-50-4P 80287-12-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction of, with telluride ion)
RN 80232-50-4 HCAPLUS

CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, 4-methylbenzenesulfonate, (2R-trans)- (9CI) (CA INDEX NAME)

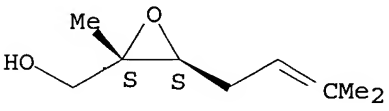


RN 80287-12-3 HCAPLUS
CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, 4-methylbenzenesulfonate, (2S-trans)- (9CI) (CA INDEX NAME)



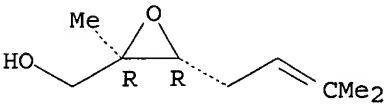
IT **80232-49-1P 80299-55-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and tosylation of)
RN 80232-49-1 HCAPLUS
CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, (2S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



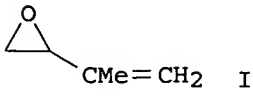
RN 80299-55-4 HCAPLUS
CN Oxiranemethanol, 2-methyl-3-(3-methyl-2-butenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L22 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:37183 HCAPLUS
DOCUMENT NUMBER: 108:37183
TITLE: Highly regioselective addition of allylstannanes to vinyl epoxides by **Lewis** acid mediation

AUTHOR(S): Naruta, Yoshinori; Maruyama, Kazuhiro
CORPORATE SOURCE: Fac. Sci., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Chemistry Letters (1987), (5), 963-6
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:37183
GI



I

AB Allylic trimethylstannes react with vinyl epoxides in the presence of BF3.OEt2 to give 1,2- or 1,4-addition products in good yield, depending on the substitution at the olefinic terminus. In either case regioselectivity is high. E.g., epoxymethylbutene I was treated with Me2C:CHCH2SnMe3 to give 91% CH2:CHCMe2CH(CH2OH)CMe:CH2, which then underwent Cope rearrangement on treatment with DBU to give 100% of a 58:42 mixture of (E)- and (Z)-HOCH2CH:CMeCH2CH2CH:CMe2.

CC 23-7 (Aliphatic Compounds)
Section cross-reference(s): 27

ST addn allylstannane vinyl epoxide regiochem; regiochem allylation vinyl epoxide; stannane allyl allylation vinyl epoxide; **Lewis** acid catalyst allylation regiochem; alkadienol; polyprenyl alc; alc unsatd

IT 1838-94-4 6705-51-7 6790-41-6 7437-61-8 **13295-59-5** 50901-75-2
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(allylation of, with allylic trimethylstannanes, regiochem. of)

IT **13295-59-5**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(allylation of, with allylic trimethylstannanes, regiochem. of)

RN 13295-59-5 HCAPLUS

CN Oxirane, 2,2-dimethyl-3-(2-methyl-1-propenyl)- (9CI) (CA INDEX NAME)